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Generalizing the Geometric Approach to Pressure Calculation
DANIEL W. SINKOVITS, Univ of Wisconsin, Stout — Pressure is the derivative of the free energy with respect to the change in volume. In a molecular dynamics simulation, there are different ways to define the infinitesimal change in volume, each corresponding to a different deformation field. The instantaneous pressure will vary depending on the choice of deformation field, but the time-average pressure should be the same for all choices. What varies is the spatial weighting of the pressure calculation. W. K. den Otter *et al.* [1] introduced this geometric approach to pressure calculation in 2001, but their thermodynamic derivation did not address time-varying deformation fields. I will use a mechanical derivation of pressure to demonstrate how to properly include a time-varying deformation field. This enables a unified understanding of the relationship between the atomic and molecular formulations of pressure. [1] W. K. den Otter, M. Kröhn, and J. H. R. Clarke, Phys. Rev. E **65**, 016704 (2001).

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